(III) Heat kernel on graphs.

In the discussion of (II.10), we see the heat kernel (and the heat semigroup) is an very useful and powerful tool to understand geometric and analytic properties of a graph. We will explore more about it in this chapter.

(III.1) Normalized heat diffusion on finite graphs.

Definition III.1.) (Heat kernel) (fundamental solution). Let $G=(V,E)$ be a finite graph. The non-negative function

$$p: V \times V \times [0,\infty) \longrightarrow [0,1]$$

is called the heat kernel, if ~~which~~ it is smooth in t, satisfies the heat equation $\frac{\partial p}{\partial t} = \Delta p$ in ~~either~~ x ~~or y~~ and satisfies $p_0(x,y) = \delta_y(x)$. □

In fact $p_t(x,y) = P_t(x,y)$ → (x,y) entry of the matrix P_t

$$= (P_t \delta_y)(x) \cancel{= P_t\delta_x(y)}.$$

By the spectral decomposition (Prop II.10.10, pp. 154), we have

$$p_t(x,y) = \sum_{i=1}^{N} e^{-\lambda_i t} \phi_i(x) \phi_i(y) d_y$$

Observe that

(1) $p_t(x,y)\, d_x = \langle P_t \delta_y, \delta_x \rangle = \langle \delta_y, P_t \delta_x \rangle$.

$$= p_t(y,x)\, d_y.$$

(2) $\forall f: V \to \mathbb{R}$, $P_t f(x) = \sum_{y\in V} P_t(f(y)\delta_y)(x) = \sum_{y\in V} f(y)\cdot (P_t\delta_y)(x)$

$$= \sum_{y\in V} p_t(x,y) f(y).$$

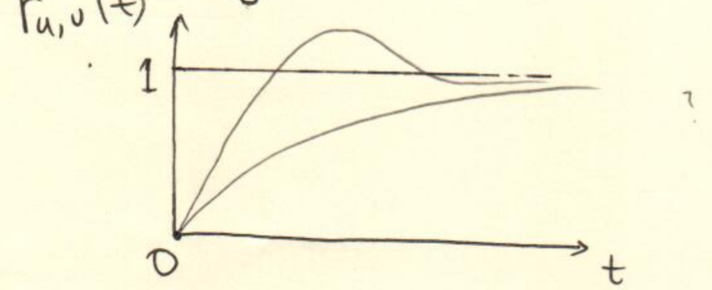
Motivation: Consider the following ratio: For any two vertices $u, v \in V$, $u \neq v$

$$r_{u,v}(t) := \frac{p_t(u,v)}{p_t(v,v)}.$$

Observe that we have

$$r_{u,v}(0) = 0, \text{ and, } \lim_{t\to\infty} r_{u,v}(t) = 1.$$

One might wonder if the function is monotonically non-decreasing?



In fact, there are graphs such that $r_{u,v}(t) > 1$ for some vertices u, v and time t: (Regev - Shinkar (2016) mentioned this was pointed out to them by Jeff Cheeger)

Prop III.1.2 Let $G=(V,E)$ be a graph. Let its eigenvalues be

$$0=\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{|V|}$$

and ϕ_i for the corresponding orthonormal eigenfunctions.

Suppose $0<\lambda_2<\lambda_3$ and $\phi_2(u) > \phi_2(v) > 0$. for some u, v.

Then $\exists\ t>0$ s.t. $r_{u,v}(t) > 1$

Proof: Recall that

$$p_t(u,v) = (P_t\delta_v)(u) = \sum_{i=1}^{|V|} e^{-t\lambda_i}\phi_i(u)\phi_i(v)d_v$$

$$= \phi_1(u)\phi_1(v)d_v + e^{-\lambda_2 t}\phi_2(u)\phi_2(v)d_v + O(e^{-\lambda_3 t})$$

And

$$P_t(u,u) = \phi_1(u)\phi_1(u)\,d_u + e^{-\lambda_2 t}\phi_2(u)\phi_2(u)\,d_u + O(e^{-\lambda_3 t})$$

where $O(\cdot)$ hides some constants that may depend on the graph, but not on t.

Recall $\phi_1 \equiv$ const, therefore

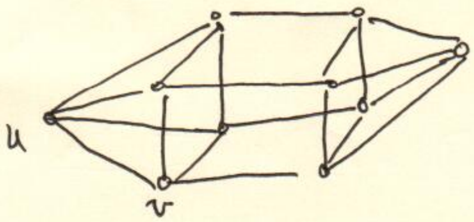
$$\phi_1(v)\phi_1(v)\,d_v = \phi_1(u)\phi_1(u)\,d_u.$$

Using the fact that $\lambda_3 > \lambda_2$ and $\phi_2(u) > \phi_2(v) > 0$, we derive for sufficiently large t,

$$r_{u,v}(t) = \frac{P_t(u,u)}{P_t(v,v)} > 1,$$

as desired. □

Therefore, $t \mapsto r_{u,v}(t)$ is can not be monotone in general.
The following examples tells ~~this~~ it is not always monotone even for
Example. (Regev - Shinkar 2016) regular graphs.



" A cube with two square pyramids attached".

It has eigenvalues $\lambda_2 = \frac{7-\sqrt{17}}{8} \doteq 0.36 < \lambda_3$.

The corresponding eigenfunction $\phi_2 = \begin{pmatrix} c \\ 1 \\ \vdots \\ 1 \\ -1 \\ \vdots \\ -1 \\ -c \end{pmatrix}$, where

$$c = 3 - \frac{7-\sqrt{17}}{2} \doteq 1.56.$$

That is, this 4-regular graph satisfies all the assumptions of Prop III.1.2.

If the heat kernel has a constant diagonal and G is regular, i.e., $p_t(u,u)d_u$ is independent of the choice of u, then we always have $r_{u,v}(t) \le 1, \ \forall t$.

This is because, for $u, v \in V$,

$$\cancel{p_t(u,v) = (P_t \delta_v)(u) = (P_{t/2} P_{t/2} \delta_v)(u)}$$

$$p_t(u,v)\, d_u = \langle P_t \delta_v, \delta_u \rangle = \langle P_{t/2} \delta_v, P_{t/2} \delta_u \rangle$$

$$= \sum_{x \in V} p_{t/2}(x,v)\, p_{t/2}(x,u)\, d_x$$

$$\le \sqrt{\sum_{x \in V} p_{t/2}(x,v)^2 d_x} \sqrt{\sum_{x \in V} p_{t/2}(x,u)^2 d_x}$$

$$= \sqrt{p_t(v,v)\, d_v} \sqrt{p_t(u,u)\, d_u}$$

The homogeneity assumption enforces

$$p_t(u,v)\, d_u \le p_t(u,u)\, d_u = p_t(v,v)\, d_v$$

That is

$$p_t(u,v) \le p_t(u,u) \Rightarrow r_{u,v}(t) \le 1.$$

Theorem III.1.3. Let $G = (V, E)$ be a regular graph. The following are equivalent:

(i) G is walk-regular: i.e, for each $l \ge 2$, the number of closed walks of length l starting and ending at a vertex is independent of the choice of the vertex.

(ii) A^l has constant diagonal for $l = 0, 1, \cdots$

(iii) Δ^l has constant diagonal for $l = 0, 1, \cdots$

(iv) P_t has constant diagonal for $t \ge 0$.

Proof: (i)$\Leftrightarrow$(ii) since $A^k(u,u)$ counts the number of closed walks of length k starting and ending at u.

(ii)$\Leftrightarrow$(iii) follows from $\Delta = D^{-1}(A-D)$ and then

$$D\Delta = A - D$$

That is $\quad d\Delta = A - dI$.

(iii)$\Rightarrow$(iv) is due to

$$P_t(u,u) = e^{t\Delta}(u,u) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} t^n \cdot \Delta^n(u,u)$$

(iv)$\Rightarrow$(iii). We have $P_t(u,u)$ is indep. of the choice of u, i.e., it can be seen as a function of t only. By uniqueness of a power series expansion, we obtain $\Delta^l(u,u)$ is indep. of u for $l = 0, 1, \ldots$. $\square$

Natural question: Is $t \mapsto r_{u,v}(t) = \frac{P_t(u,v)}{P_t(u,u)}$, $u \neq v$, monotone for walk-regular graphs?

Walk regular graphs include

(a) vertex transitive graphs: Given any two vertices u and v, $\exists$ an automorphism $f: G \to G$ s.t. $f(u) = f(v)$. That is, its automorphism group acts transitively on its vertices.

(b) distance-regular graphs: a regular graph s.t. for any two vertices u and v, the number of vertices that are at distance j from u and at distance k from v only depends only on j, k, and $i = \text{dist}(u,v)$.

Rmk: • One can directly show that any distance-regular graph ~~have~~ satisfies Thm III.1.3. (ii).

• A distance-regular graph is not necessarily vertex-transitive. A small example is the Chang graphs: (张里千, Li-Chien Chang)
They are the 3 graphs with 28 vertices. Actually they're strongly regular graphs with parameter (28, 12, 6, 4)
van Dam and J. H. Koolen (库仑) ~~sho~~ constructed a family of non-vertex transitive distance-regular graphs with unbounded diameter. (Invent. Math. 2005)

(c). Regular graphs with at most 4 distinct eigenvalues.

Rmk: For regular graph with s distinct eigenvalues, there exists a monic polynomial p of degree $s-1$, s.t. the matrix $p(A)$ has constant entries.
This polynomial is called Hoffman polynomial of G.
Therefore, walk regularity of such a regular graph G with s distinct eigenvalues is equivalent to

$$A^l \text{ having const. diagonal}, \quad l = 0, \dots, s-2.$$

Clearly, A^0, A, A^2 have const. diagonal. Therefore, regular graphs with ≤ 4 distinct eigenvalues are walk regular.

Progress:

(1). ~~Shink~~ Regev - Shinkar 16. counter example ~~in the~~ which is a Cayley graph. A Cayley graph is vertex transitive. In fact, Peres (2013) ~~ask~~ ~~or~~ asked

- Is the function $t \mapsto r_{u,v}(t)$ monotonically non-decreasing in t for all vertex transitive graphs and all vertices u, v?

Regev - Shinkar '16 give a negative answer.

(2). Price '17 ~~show~~ answer Peres' question positively for ~~a~~ finite abelian Cayley graphs!

Natural question: What happens for vertex transitive graphs satisfying $CD(0, \infty)$?

or ~~s~~ strengthen it to be optimal lower curvature bound $= 0$.

We remark that all abelian Cayley graphs satisfy $CD(0, \infty)$.

(3). Nica '20. show $r_{u,v}$ is monotonically non-decreasing for regular graphs with 3 distinct eigenvalues.

(4) Kubo - Namba '21 show $r_{u,v}$ is monotonically non-decreasing for regular bipartite graphs with 4 distinct eigenvalues?

Question: Can one drop "bipartiteness"?

We will discuss Nica's result in details.

The following Lemma is a preparation.

Lemma III.1.4. Let $G = (V,E)$ be a d-regular non-complete graph. Then

$$\lambda_2 \le 1 \quad \text{and} \quad \lambda_N \ge \frac{d+1}{d}.$$

<u>Proof</u>: $\lambda_2 \le 1$ has been shown in pp. 23.

$\lambda_N \ge \frac{d+1}{d}$ is a result due to Grone–Merris.

Note $K_{1,d}$ is a subgraph of G. (not necessarilly an induced subgraph).

Recall the largest eigenvalue of $K_{1,d}$ is $\frac{1+d}{d}$.

The estimate follows from the <u>interlacing</u> theorem. □